Institution: The University of Manchester

Unit of Assessment: UoA9 Physics

Title of case study: CPO software package for designing charged-particle optical systems.

1. Summary of the impact

A software package called CPO has been developed that simulates the motion of charged particles in electromagnetic fields. More than 200 benchmark tests have established CPO as the gold standard in low-energy charged-particle optics. A spin-off company was formed to market CPO, [text removed for publication]

2. Underpinning research

The key researchers were:

Prof. F. H. Read, FRS, (Head of Research Group, 1993-2005 and Emeritus thereafter).
Dr N. J. Bowring (Senior Experimental Officer, 1993-2002, and collaborations thereafter).
Prof. G.C. King (Sen. Lect., 1993-5; Reader, 1995-01; Prof. of Physics, 2001-07 and Emeritus thereafter).
Prof. A. J. Murray (Lect. 1999-01; Sen. Lect. 2001-02; Reader 2002-07; Prof. of Physics, 2008-date).

The impact is based on research undertaken in atomic and molecular physics during the period 1993 to the present, which in that time produced >150 peer-reviewed publications with > 40 publications on electron optics and associated instrumentation. As part of the research programme, a software package called Charged Particle Optics (CPO) was developed to simulate the motion of charged particles in electrostatic and magnetic fields; see [5] for a recent description. Underpinning this research was the development of a three-dimensional technique, which employs the *Boundary Element* (BE) method for solving electromagnetic problems rather than conventional *Finite Element* (FE) or *Finite Difference* (FD) methods. This BE method is one or two orders of magnitude more accurate than FE or FD methods for the same computing time [5]. Other advantages of CPO software are that it can deal with electrodes of essentially any shape and it is particularly powerful for space-charge problems such as electron guns. In the course of the research, CPO was also developed to handle magnetic fields as well as electrostatic fields.

The use of CPO led to the following key advances: (i) the design of electrostatic lenses with very low aberrations, which was achieved through the high accuracy in modelling electron trajectories, (ii) the development of high-current electron guns, which exploited the ability of CPO to include the effects of Coulomb interactions between charged particles [3], (iii) the optimisation of three-dimensional electron optical devices [2] and (iv) the invention of new electron optical devices [1]. A good example of this is the invention of the *magnetic angle-changer*. This enabled for the first time, electrons that are scattered from a gaseous target be detected over the full range of scattering angle, from 0 to 180°, [4,6]. This enabled theory to be tested in regions that were previously inaccessible to experiment and provided the most accurate values of scattering cross-sections that are of practical importance. The magnetic angle-changer was described by an international conference speaker [text removed for publication] as “the most important development in low-energy electron spectroscopy in 25 years”.

3. References to the research

The research has been published in leading journals including; Physical Review Letters, Journal of Physics B: Atomic, Molecular and Optical Physics and Review of Scientific Instruments. The publications have been cited on numerous occasions; for example, refs. [1] and [4] have been cited 94 and 61 times respectively, according to *Web of Knowledge*. The research has also been presented at international conferences including the: *International Conference on Photonic, Electronic & Atomic Collisions* and *International conference on Charged Particle Optics*.

Key references

[1] “Production and optical properties of an unscreened but localized magnetic field”, Read F. H. and Channing J., Rev. Sci. Instrum., 67, 1996, 2372-7, (1996). DOI: 10.1063/1.1147004

[2] “Accurate Monte-Carlo calculation of Boersch energy and angle spreading”, Read F.H. and Bowring N.J., Rev. Sci. Instrum., **74**, 2280, (2003). DOI:10.1063/1.1544422

[3] “The parallel cylindrical mirror electron energy analyser”, Read F.H., Rev. Sci. Instrum., **73**, 1129, (2002). DOI: 10.1063/1.1435841

Other References

[4] "Measurements of elastic electron scattering in the backward hemisphere", Zubek M., Gulley N., King G.C. and Read F.H., J. Phys. B Atom. Molec. Phys, 29, L239, (1996). DOI: 10.1088/0953-4075/29/6/011

[5] "The CPO programs and the BEM for charged particle optics", Read F.H. and Bowring N.J., Nucl. Instrum. Meths. in Phys. Res., 654, 273, (2011). DOI:10.1016/j.nima.2010.12.163

[6] "Super-elastic scattering from calcium over the complete angular scattering range using a magnetic angle changing device." Hussey M., Murray A.J., MacGillivary W.R., and King G.C., Phys. Rev. Letts. 99, 133202, (2007). DOI: 10.1103/PhysRevLett.99.133202

4. Details of the impact

Research in atomic and molecular physics at Manchester requires state-of-the-art instrumentation for the study of atoms and molecules by electron spectroscopy. This requires accurate knowledge of the behaviour of electrons and ions in the electrostatic and magnetic fields of the instrumentation. Consequently, a software package (CPO) was developed to model this behaviour precisely. Analytical instruments using charged-particle optics are also widely used in industry. These instruments also need to have the highest performance for the increasingly demanding requirements of customers. Consequently, a spin-off company was formed to make CPO available to manufacturers of scientific instruments and other users of electron optics. This company, called Charged Particle Optics Ltd, was started by two staff from the School of Physics and Astronomy (Read & Bowring).

The principle advantage of CPO for customers is that it is one or two orders of magnitude more accurate than conventional finite element or finite difference methods. This has been demonstrated by more than 200 benchmark tests that are based on problems that have well known analytical solutions. These benchmark tests are readily available to prospective customers, [A] and these tests have established CPO as the gold standard of charged particle optics. This superior accuracy provides, for example, enhanced mass resolution in a mass spectrometer [text removed for publication]. Other important advantages are that CPO can easily deal with electrodes of any shape and of very different sizes, such as nano-sized electrodes in centimetre-sized systems, and because CPO is a charge-based method, it can deal with systems that include space charge and/or cathodes. These are of crucial importance to manufactures of high throughput analysis tools, [text removed for publication] . Moreover, a manufacturer can use CPO to develop and test designs for new products before any metal is machined, saving them considerable time and cost [text removed for publication].

CPO has been sold [text removed for publication].

Illustrative Examples of Impact

(i) [text removed for publication].

(ii) [text removed for publication]

(iii) At the Jet Propulsion Laboratory (JPL), California, CPO was used to simulate the electron ionizer in the prototype of a gas chromatographic mass spectrometer system that was later flown as a flight version to the International Space Station (ISS). The purpose of this instrument is to monitor the concentration – at the parts-per-million to parts-per-billion levels – of trace, toxic chemical species in the ISS cabin atmosphere. Species include acetone, ethanol, aldehydes, ketones, benzene, and perfluoropropane. The unit also monitors the major constituent species N_2, O_2, CO_2, and Ar. Both types of measurements are needed to assure astronaut safety in the cabin. All data are processed on-board by the instrument, and as well transmitted to JPL for further analysis and archiving. The full space-charge capability of CPO was especially important to the design and testing of the electron ionizer of the mass spectrometer. [text removed for publication] The instrument was used successfully for two years aboard the Space Station, and was recently returned to Earth for refurbishment [text removed for publication].

Summary of Economic Impact

[text removed for publication]

5. Sources to corroborate the impact

[A] Information about CPO, benchmark tests and prices from: Charged Particle Optics programs

web site: http://www.electronoptics.com/.

[B] [text removed for publication]

[C] [text removed for publication]

[D] [text removed for publication]

[E] [text removed for publication].